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Superconductivity and spin triplet collective mode in the $t-J$ model close to antiferromagnetic instability

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Abstract

To investigate relations between long-range antiferromagnetic (AF) order, superconductivity and two particle triplet collective excitations we consider a modified two dimensional $t-J$ model at doping close to half filling. The model includes additional hopping t'' and nearest sites Coulomb repulsion V. The additional parameters allow us to control closeness of the system to the AF instability. We demonstrate the possibility of co-existence of long-range AF order and d-g-wave superconductivity. In the phase with long-range AF order we find, analytically, superconducting gaps and spin wave renormalization. We demonstrate that at approaching the point of the AF instability the spin triplet collective excitation arises with energy below the superconducting gap.

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It is widely accepted now that superconductivity of cuprates is closely related to their unusual magnetic properties, and it is increasingly clear that magnetic pairing is the most realistic mechanism of cuprate superconductivity. However the mechanism of pairing as well as other unusual properties are far from completely understood. The problem has been attacked along several directions. First we have to mention the empirical or semi-empirical approach which allows one to relate different characteristics measured experimentally. This approach is to a large extent based on the Hubbard model. For a review see article[1]. In the low energy limit, the Hubbard model can be reduced to the $t-J$ model. Another approach to cuprates is based on numerical studies of the $t-J$ model (see review[2]). Our studies are also based on this model. We used the ordered Neel state at zero doping as a starting point to develop spin-wave theory of pairing[3]. The method we used was not fully satisfactory, since it violated spin-rotational symmetry, nevertheless it allowed us to calculate from first principles all the most important properties including critical temperature, spin-wave pseudogap and low energy spin triplet excitations[4].

A sharp collective mode with very low energy has been revealed in YBCO in spin polarized inelastic neutron scattering[5–7]. A number of theoretical explanations have been suggested for this effect[8,4]. All of those explanations are based on the idea that the system is close to AF instability. However, all known explanations use some uncontrolled approximations and assumptions.

In the present work we investigate a close to half filling regime for the 2D $t-J$ model where it can be solved analytically without any uncontrolled approximations. It can be done for the region of parameters where long-range AF order is preserved under doping. We analyze the superconducting pairing in this regime and consider spin triplet collective excitation. It is demonstrated that the narrow collective mode arises at approaching the point of AF instability and the energy of the mode is below the superconducting gap.

Let us consider a $t-J-J''-V$ model defined by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - t'' \sum_{\langle ij_2 \rangle \sigma} c^\dagger_{i\sigma} c_{j_2\sigma} + \sum_{\langle ij \rangle} \left[J \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j \right) + V n_i n_j \right]. \quad (1)$$

$c^\dagger_{i\sigma}$ is the creation operator of an electron with spin σ ($\sigma =\uparrow,\downarrow$) at site i of the two-dimensional square lattice. The $c^\dagger_{i\sigma}$ operators act in the Hilbert space with no double electron occupancy. The $\langle ij\rangle$ represents nearest neighbor sites, and $\langle ij_2\rangle$ represents next next nearest sites. The spin operator is $\mathbf{S}_i = \frac{1}{2}\sum_{\alpha,\beta} c^\dagger_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}$, and the number density operator is $n_i = \sum_\sigma c^\dagger_{i\sigma}c_{i\sigma}$. In addition to the minimal $t-J$ model (see Ref.[2]) we have introduced additional next next nearest hopping t'', and Coulomb repulsion V at nearest sites. Note that we do not introduce next nearest neighbor hopping t' (diagonal) because we do not need it for the purposes of this study.

In the present work we consider the perturbation theory limit $t, t'' \ll J$. It is well known that the $t-J$ model with small hopping has phase separation at doping. The reason for this is very simple: attraction between holes at nearest sites due to the reduction in number of missing AF links. The value of this attraction immediately follows from eq.(1): $U \approx J\langle \mathbf{S}_i\mathbf{S}_j - 1/4\rangle \approx -0.58J$. This effect is very simple and is not of interest to us. To overcome it we choose a Coulomb repulsion $V = 0.58J$. So the only purpose of introducing the Coulomb repulsion in the model is to eliminate short range hole-hole attraction.

We consider phase with long range AF order. It is well known (see e.g. Ref.[9]) that minima of the single hole dispersion are at the faces of the magnetic Brillouin zone $(\pm\pi/2, \pm\pi/2)$, and the dispersion is (we take energy at the minimum as a reference point)

$$\begin{aligned} \epsilon_k &= \beta_1\gamma_{\mathbf{k}}^2 + \beta_2(\gamma_{\mathbf{k}}^-)^2, \\ \beta_1 &= 3.26t^2/J + 8t'', \quad \beta_2 = 1.21t^2/J + 8t''. \end{aligned} \tag{2}$$

$\gamma_{\mathbf{k}} = \frac{1}{2}(\cos k_x + \cos k_y)$, $\gamma_{\mathbf{k}}^- = \frac{1}{2}(\cos k_x - \cos k_y)$. Calculation of the t'' contribution in the dispersion (2) is straightforward because it is hopping within the same magnetic sublattice. Calculation of the t-contribution is more complicated, and we use the results of a series expansion[10]. Note that a selfconsistent Born approximation[11] gives substantially different coefficients ($\beta_1 = 1.86t^2/J$, $\beta_2 = 0.26t^2/J$). The reason is that there are several important diagrams at small t which are missed in this approximation. We will consider the case of very small doping, $\delta \ll 1$, with respect to half filling (total filling is $1-\delta$). In this case

all holes are concentrated in small pockets around the points $\mathbf{k_0} = (\pm\pi/2, \pm\pi/2)$. Single hole dispersion (2) can be expanded near each of these points $\epsilon_k = \beta_1 p_1^2/2 + \beta_2 p_2^2/2$, where $\mathbf{p}$ is deviation from the center of the pocket: $\mathbf{p} = \mathbf{k} - \mathbf{k_0}$, p_1 is orthogonal to the face of the magnetic Brillouin zone, and p_2 is parallel to the face. The Fermi energy and Fermi momentum for the holes equal $\epsilon_F \approx \frac{1}{2}\pi(\beta_1\beta_2)^{1/2}\delta$, $p_F \approx \sqrt{p_{1F}p_{2F}} \approx (\pi\delta)^{1/2}$.

Spin-wave excitations on an AF background are usual spin waves with dispersion $\omega_{\mathbf{q}} = 2J\sqrt{1-\gamma_{\mathbf{q}}^2} \approx \sqrt{2}Jq$, at $q << 1$, see Ref.[12] for review.The hole-spin-wave interaction is well known (see, e.g. Ref.[11])

$$H_{h,sw} = \sum_{\mathbf{k},\mathbf{q}} g_{\mathbf{k},\mathbf{q}} \Big(h^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} h_{\mathbf{k}\uparrow} \alpha_{\mathbf{q}} + h^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} h_{\mathbf{k}\downarrow} \beta_{\mathbf{q}} + \text{H.c.} \Big), \tag{3}$$
$$g_{\mathbf{k},\mathbf{q}} = 4t\sqrt{2}(\gamma_{\mathbf{k}} U_{\mathbf{q}} + \gamma_{\mathbf{k}+\mathbf{q}} V_{\mathbf{q}}),$$

where $h^\dagger_{\mathbf{k}\sigma} = c_{\mathbf{k},-\sigma}$ is the hole creation operator, $\alpha^\dagger_{\mathbf{q}}$ and $\beta^\dagger_{\mathbf{q}}$ are the spin wave creation operators for $S_z = \mp 1$, and $U_{\mathbf{q}} = \sqrt{\frac{J}{\omega_{\mathbf{q}}} + \frac{1}{2}}$ and $V_{\mathbf{q}} = -sign(\gamma_{\mathbf{q}})\sqrt{\frac{J}{\omega_{\mathbf{q}}} - \frac{1}{2}}$ are parameters of the Bogoliubov transformation diagonalizing spin-wave Hamiltonian, see Ref.[12]. To describe renormalization of the spin wave under doping, it is convenient to introduce the set of Green's functions[13]

$$D_{\alpha\alpha}(t,\mathbf{q}) = -i\langle T[\alpha_{\mathbf{q}}(t)\alpha^\dagger_{\mathbf{q}}(0)]\rangle, \tag{4}$$
$$D_{\alpha\beta}(t,\mathbf{q}) = -i\langle T[\alpha_{\mathbf{q}}(t)\beta_{-\mathbf{q}}(0)]\rangle,$$
$$D_{\beta\alpha}(t,\mathbf{q}) = -i\langle T[\beta^\dagger_{-\mathbf{q}}(t)\alpha^\dagger_{\mathbf{q}}(0)]\rangle,$$
$$D_{\beta\beta}(t,\mathbf{q}) = -i\langle T[\beta^\dagger_{-\mathbf{q}}(t)\beta_{-\mathbf{q}}(0)]\rangle.$$

In the present work we consider only the long-range dynamics: $q \sim k \sim p_F \ll 1$. In this limit all possible polarization operators coincide[4] $P_{\alpha\alpha}(\omega,\mathbf{q}) = P_{\alpha\beta}(\omega,\mathbf{q}) = P_{\beta\alpha}(\omega,\mathbf{q}) = P_{\beta\beta}(\omega,\mathbf{q}) = \Pi(\omega,\mathbf{q})$. For stability of the system the condition (Stoner criterion)

$$\omega_q + 2\Pi(0,\mathbf{q}) > 0 \tag{5}$$

must be fulfilled[14]. Otherwise the Green's functions (4) would possess poles with imaginary ω. Considering holes as a normal Fermi liquid one can easily calculate the polarization

operator at $q \ll p_F$: $\Pi(0,\mathbf{q}) \approx -4t^2\sqrt{2}q/\pi\sqrt{\beta_1\beta_2}$, Ref.[14]. Relatively weak pairing, which we consider below, does not influence this result. Then the condition of stability can be rewritten as

$$\sqrt{\beta_1\beta_2} > \frac{8t^2}{\pi J}. \tag{6}$$

The dispersion (2) at $t'' = 0$ violates this condition. This is a well known statement about the instability of long-range AF order under doping in a pure $t - J$ model. To provide stability we have to choose $t'' > t''_c = 0.0635t^2/J$. We want to have the system in the phase with long range AF order, but close to the point of instability, and therefore we will consider t'' only slightly above the critical value. As a measure of this closeness it is convenient to introduce the parameter η

$$\eta^2 = 1 - \frac{8t^2}{\pi J\sqrt{\beta_1\beta_2}} \approx 3.4\frac{J(t'' - t''_c)}{t^2} \ll 1. \tag{7}$$

The criterion (5) is proportional to this parameter.

Superconducting pairing mediated by the spin-wave exchange can be found analytically[3]. Only the pairing within one pocket is important. There is no solution for the gap without nodes (s-wave), and there is an infinite number of solutions with the nodes. The pairing is maximum for the case of a single node line in the pocket, and the gap at the Fermi surface ($\epsilon_F = \beta_1 p_1^2/2 + \beta_2 p_2^2/2$) is of the form

$$\Delta(\phi) = \Delta_0 \sin\phi, \tag{8}$$
$$\Delta_0 = C\epsilon_F e^{-1/g},$$

where

$$\sin\phi = \frac{\sqrt{\beta_2}p_2}{\sqrt{\beta_1 p_1^2 + \beta_2 p_2^2}}, \tag{9}$$
$$g = \frac{8t^2}{\pi J\beta_2(\sqrt{\beta_1/\beta_2} + 1)^2},$$

and $C \sim 1$ is some constant. Energy spectrum and Bogoliubov parameters are given by the usual BCS formulas

$$E_{\mathbf{k}} = \sqrt{(\epsilon_k - \epsilon_F)^2 + \Delta_{\mathbf{k}}^2}, \tag{10}$$
$$u_{\mathbf{k}}^2, v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 \pm \frac{\epsilon_{\mathbf{k}} - \epsilon_F}{E_{\mathbf{k}}}\right)$$

Substituting values $\beta_1 = 3.77t^2/J$ and $\beta_2 = 1.78t^2/J$ corresponding to the critical point, we find $g \approx 0.25$, and hence

$$\Delta_0 \approx \epsilon_F e^{-4} \approx 0.07\frac{t^2\delta}{J}. \tag{11}$$

The eqs.(8),(9), and (11) describe pairing within a single pocket. There are effectively two pockets in the magnetic Brillouin zone. Taking symmetric and antisymmetric combinations between pockets we get d- and g-wave pairings respectively (see Ref.[3] for details). The gaps, as well as the critical temperatures for d- and g-wave, are practically the same. Note that we discuss the situation without short range hole-hole interaction, which has been eliminated by adjusting the nearest sites hole-hole Coulomb repulsion ($V \approx 0.58J$, see above). If one destroys this adjustment, the degeneracy between d- and g-waves is also destroyed. The crucial point is that the g-wave is not sensitive at all to the interaction at nearest sites, whereas the d-wave is very sensitive. Therefore at $V < 0.58J$ the d-wave pairing is enhanced, while on the contrary, at larger Coulomb repulsion $V > 0.58J$ the d-wave is suppressed and disappears very fast.

Now we can discuss the spectrum of the spin-triplet excitations. The Spin wave polarization operator due to the mobile holes is of the form (see e.g. Ref.[4])

$$\Pi(\omega, \mathbf{q}) = \sum_{\mathbf{k},\mathbf{k_0}} g_{\mathbf{k_0 q}}^2 \frac{2(E_{\mathbf{k}} + E_{\mathbf{k+q}})}{\omega^2 - (E_{\mathbf{k}} + E_{\mathbf{k+q}})^2}\left(u_{\mathbf{k}}^2 v_{\mathbf{k+q}}^2 + u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k+q}} v_{\mathbf{k+q}}\right). \tag{12}$$

It accounts for both normal and anomalous fermionic Green's functions. Eq. (12) includes summation over pockets $\mathbf{k_0} = (\pi/2, \pm\pi/2)$. In these pockets the vertex is $g_{\mathbf{k_0,q}} \approx 2^{5/4}t(q_x \pm q_y)/\sqrt{q}$. Let us consider the case of very small momenta and frequencies: $v_F q < \Delta_0$, and $\omega < \Delta_0$. In this limit one can put $q = 0$ in eq. (12) everywhere except at the vertex and therefore the polarization operator can be evaluated analytically

$$\Pi(\omega, \mathbf{q}) = -\frac{4t^2\omega_{\mathbf{q}}}{\pi J\sqrt{\beta_1\beta_2}}\left(1 + i\frac{\pi\omega}{8\Delta_0}\right) \tag{13}$$

Note that the the imaginary part is nonzero even at $\omega < 2\Delta_0$ because the gap (8) has a line of nodes. Any of the Green's functions (4) have a denominator $\omega^2 - \omega_{\mathbf{q}}^2 - 2\omega_{\mathbf{q}}\Pi(\omega, \mathbf{q})$, see e.g. Refs.[13,4]. The zero of this denominator gives the energy and width of the spin-triplet collective excitation. Using eqs.(13) and (7) we find

$$
\begin{aligned}
o_{\mathbf{q}} &= \eta\omega_{\mathbf{q}}, \\
\Gamma_{\mathbf{q}} &= \frac{\pi\omega_{\mathbf{q}}}{8\Delta_0} o_{\mathbf{q}}.
\end{aligned}
\tag{14}
$$

In essence this is the renormalized spin-wave, but its energy is much smaller than the energy of the bare spin-wave, $o_{\mathbf{q}}/\omega_{\mathbf{q}} = \eta \ll 1$. This collective excitation exists as a narrow peak only at very small q when $\pi\omega_{\mathbf{q}}/8\Delta_0 < 1$. At higher q the width is larger than its frequency because of decay to particle hole excitations.

The last question we want to discuss is how close to the point of AF instability can we approach using the present description, or in other words how small can η be? The superconducting pairing itself is not sensitive to the AF instability and it survives at the transition to the disordered phase. The reason for this is clear: even in the disordered phase the magnetic correlation length ξ_M is much larger than the typical distances $r \sim 1/p_F \sim 1/(\pi\delta)^{1/2}$ which are important for pairing. However the spin-triplet spectrum (14) is valid only if η is not too small. The sublattice staggered magnetization m is renormalized because of spin-wave spectrum renormalization, see Ref.[4]

$$
\delta m = -2J \int \left(\frac{1}{o_{\mathbf{q}}} - \frac{1}{\omega_{\mathbf{q}}} \right) \frac{d^2q}{(2\pi)^2}. \tag{15}
$$

The integral converges at the momenta q where the collective excitation exists as a narrow mode: $q < \Delta_0/J$. Our consideration is valid if the renormalization of staggered magnetization is small: $\delta m \ll 0.5$. Together with eq. (15) this gives the limit for validity of our approach.

$$
\eta \gg \Delta_0/J \tag{16}
$$

At $\Delta_0 > \eta/J > 0$ equation (14) for the spectrum is not valid, but nevertheless there is some

gapless spin-triplet excitation. The point $\eta = 0$ indicates transition to the spin liquid phase and a spin-wave gap is opened here.

In conclusion we have considered a close to half filling $t-J-J''-V$ model with Coulomb repulsion $V = 0.58J$ adjusted to eliminate short range hole-hole interaction. We restrict our consideration by the case of small t, $t \ll J$, and small doping $\delta \ll 1$. It is demonstrated that at $t'' > 0.0635t^2/J$ the Neel order is preserved under the doping, and at $t'' < 0.0635t^2/J$ the order is destroyed and the system undergoes transition to the spin liquid phase. In both phases there is d-g-wave superconducting pairing mediated by spin-wave excitations. In the Neel state we found, analytically, collective spin triplet excitation. It exists as a narrow mode only at very small momenta and its energy is substantially below the energy of the bare spin wave.

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